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The Defective Structure of Excess-Ca Dolomite

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Diffraction features observed for non-stoichiometric excess-Ca dolomite samples from Eocene rocks of the Floridan aquifer and from Permian rocks of New Mexico demonstrate the presence of defect structures. The X-ray diffraction patterns recorded using synchrotron and Cu Kα radiation contain two types of reflections in the form of sharp, narrow Bragg lines and diffuse maxima. The intensity of the Bragg reflections decrease more than expected with increasing 2θ angle, while the intensity of the diffuse maxima increases as a consequence of the structural modifications arising from compositional heterogeneity. The observed diffraction features are analyzed based on the theory of X-ray diffraction in nonideal crystals.

It is shown that both the Bragg and diffuse reflections belong to a single defective structure. It was assumed that the dolomite microcrystals in the samples contain structural distortions as a result of compositional heterogeneity in which high-excess-Ca dolomite microcrystals contain small domains of low excess Ca. These domains create long-range atomic displacements. A modified Rietveld method was used to refine the average structures of both the high-excess-Ca and low-excess-Ca components of these samples. It was found that the A sites in both structures are occupied by Ca, whereas the excess Ca is located in the B site. The refined interatomic distances for the average structure are consistent with site occupancies and ionic radii. The findings are related to previous transmission electron microscopy studies showing the existence of defective domains. A possible physical model of the defective structure of the studied excess-Ca dolomite samples is discussed.

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